1,2,3-Trichloropropene

96-19-5 | DTXSID3047766

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -29.6 °C

Global applicability domain: Inside

Local applicability domain index: 7.16e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

Image not found
1-Propene, 3,3,3-trichloro-
Measured: -30.0
Predicted: -51.7

Image not found
Propane, 1,2,3-tribromo-
Measured: 16.9
Predicted: 8.98e-01

Image not found
1,2,3-Trichloropropane
Measured: -14.7
Predicted: -33.1

Image not found
(Z)-1,2-Dichloroethylene
Measured: -64.9
Predicted: -69.7

Image not found
(E)-1,2-Dichloroethylene
Measured: -64.9
Predicted: -69.7

Image not found
1,2-Dichloroethylene
Measured: -57.0
Predicted: -69.7